

3,3'-Dichlorobenzidine  
91-94-1 | DTXSID6020432

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $3.49 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.73 \times 10^{-1}$

**Confidence level:**  $6.93 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2-Methyl-p-benzoquinone

**Measured:**  $2.35 \times 10^{-11}$

**Predicted:**  $2.15 \times 10^{-11}$

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1,4-Benzoquinone

**Measured:**  $4.60 \times 10^{-12}$

**Predicted:**  $5.97 \times 10^{-12}$

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1,3,5-Cycloheptatriene

**Measured:**  $9.69 \times 10^{-11}$

**Predicted:**  $1.00 \times 10^{-10}$